
AFRL-OSR-VA-TR-2014-0078

# DATABASES FOR THE GLOBAL DYNAMICS OF MULTIPARAMETER NONLINEAR SYSTEMS

**Konstantin Mischaikow**
**RUTGERS THE STATE UNIVERSITY OF NEW JERSEY**

**03/05/2014**
**Final Report**



Air Force Research Laboratory
AF Office Of Scientific Research (AFOSR)/ RTC
Arlington, Virginia 22203
Air Force Materiel Command

# REPORT DOCUMENTATION PAGE

*Form Approved*
*OMB No. 0704-0188*



**PLEASE DO NOT RETURN YOUR FORM TO THE ABOVE ORGANIZATION.**

| 1. REPORT DATE *(DD-MM-YYYY)* | 2. REPORT TYPE | 3. DATES COVERED *(From - To)* |
|---|---|---|
| 28/02/2014 | Final | 03/01/2009 - 11/30/2013 |

**4. TITLE AND SUBTITLE**

Databases for the Global Dynamics of Multiparameter Nonlinear Systems

**5a. CONTRACT NUMBER**

**5b. GRANT NUMBER**

FA9550-09-1-014

**5c. PROGRAM ELEMENT NUMBER**

**6. AUTHOR(S)**

Konstantin Mischaikow

**5d. PROJECT NUMBER**

**5e. TASK NUMBER**

**5f. WORK UNIT NUMBER**

**7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)**

Rutgers, The State University of New Jersey
ASB III, Rutgers Plaza
New Brunswick, NJ 08807

**8. PERFORMING ORGANIZATION REPORT NUMBER**

**9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)**

Air Force Office of Scientific Research

**10. SPONSOR/MONITOR'S ACRONYM(S)**

AFOSR

**11. SPONSOR/MONITOR'S REPORT NUMBER(S)**

**12. DISTRIBUTION/AVAILABILITY STATEMENT**

Approved for Public Release

**13. SUPPLEMENTARY NOTES**

**14. ABSTRACT**

Developed mathematical theory, efficient algorithms (both with respect to time and memory) and open access code to obtain a rigorous database for the global dynamics of multiparmeter nonlinear systems. This included the development of efficient algorithms and open access code for computing homological invariants. These tools were applied to a variety of systems including network models from biology and the analysis of complex spatio-temporal patterns arising in condensed matter physics.

**15. SUBJECT TERMS**

Nonlinear Dynamics, Computational Topology, Topological Data Analysis

| 16. SECURITY CLASSIFICATION OF: | | | 17. LIMITATION OF ABSTRACT | 18. NUMBER OF PAGES | 19a. NAME OF RESPONSIBLE PERSON |
|---|---|---|---|---|---|
| a. REPORT | b. ABSTRACT | c. THIS PAGE | | | Konstantin Mischaikow |
| | | | | | 19b. TELEPHONE NUMBER *(Include area code)* 848-445-6980 |

# DATABASES FOR THE GLOBAL DYNAMICS OF MULTIPARAMETER NONLINEAR SYSTEMS
# FA9550-09-1-0148
# Final Report

Konstantin Mischaikow
Department of Mathematics/BioMaPS Institute
Rutgers University

The goal of this project was the development of a rigorous, efficiently computable, finite algebraic/combinatorial description of global dynamics applicable to multi parameter nonlinear dynamical systems. We refer to the output as a Database for Global Dynamics since it allows the user to query for information about the existence and structure of dynamics at either a given parameter value or over sets of parameter values.

The following individuals at Rutgers were directly involved in carry out research associated with this project.

- Konstantin Mischaikow, Professor, PI
- Shaun Harker, Research Scientist
- Miro Kramar, Postdoctoral Fellow
- Jay Mireles-James, Postdoctoral Fellow
- Amit Patel, Postdoctoral Fellow
- Arnaud Goullet, Postdoctoral Fellow
- Vidit Nanda, Graduate Student
- Justin Busch, Graduate Student
- Kelly Spendlove, Graduate Student
- Rachel Levanger, Graduate Student
- Jonathan Jaquette, Undergraduate Student

- Daniel Weingard, Undergraduate Student

The work and associated results can be divided into the following overlapping topics.

1. *Discretization of phase space and parameter space.* The fact that grids of arbitrarily small diameter exist for any compact metric space [7] implies that, at least theoretically, the Database can be constructed for any continuous dynamical system defined on a compact metric space. However, the first step in implementation requires a data structure for the grids. If the dynamical system is defined on $\mathbb{R}^n$, then cubical grids appear to be an optimal choice. However, if the dynamical system is defined on a manifold, then we need to use charts. The most recent version of the database software [15] supports a discretization modeled after stratified spaces. We also began to investigate the implementation of the Database algorithms on complexes generated by time series data.

2. *Approximation of maps.* The results of the database are rigorous if one has an outer approximation of the underlying nonlinear map. Given an analytic representation of map that generates the dynamics, the most straightforward means of ensuring an outer approximation is to use interval arithmetic [1]. However, this leads to large over estimates and hence to weaker characterizations of the global dynamics. The most recent version of the database software [15] has a module that accesses the map and produces that outer approximation. Thus it allows us to vary the methods used to obtain an outer approximation. In particular we are no longer bound to use interval vectors [2]. We also began to study the feasibility of constructing outer approximations based on time series data and obtained probabilistic results concerning the ability to reconstruct the homotopy of a map from random data points [3].

3. *Identification of recurrent and gradient-like dynamics.* Successful application of topics 1 and 2 lead to the following methodology for identify the regions of phase space which contain gradient-like dynamics versus those regions of phase space which may contain recurrent dynamics:

   (a) We form a discretization $\mathcal{G}$ of phase space.

   (b) We create a multi-valued map $\mathcal{F} : \mathcal{G} \rightrightarrows \mathcal{G}$ which is an outer-approximation of an underlying continuous map $f$.

   (c) We construct a directed graph $G = (V, E)$ which represents $\mathcal{F}$ by letting the nodes of $G$ be represent grid elements of $\mathcal{G}$ and the directed edges represent the information in $\mathcal{F}$.

   (d) We compute the *Strongly Connected Path Components* (SCPC's) of $G$.

   (e) We realize the computed SCPC's as isolating neighborhoods of the underlying dynamics.

Strongly Connected Path Components may be computed by computing Strongly Connected Components (the concepts are almost identical). The traditional way to compute this is to utilize an algorithm called *Tarjan's algorithm*. This algorithm is linear time, and one cannot expect to do any better time-wise. (Unless one wishes to find a parallel algorithm. We have not done this, and it is a very difficult open problem how to compute strong components efficiently in parallel.) The difficulty we face is memory requirements. Because we have a formula for $\mathcal{F}$, we should like to store the graph $G$ without explicitly storing the edges, which may be so numerous as to easily overwhelm our memory limits. One could simply recompute out-edges whenever they were needed, but this results in very long running times, as the computation of out-edges is the time-consuming aspect of the algorithm.

We have developed a variant of Tarjan's algorithm" which need only calculate the out-edges of a node a single time, but requires only $\mathcal{O}(|V|)$ space as opposed to $\mathcal{O}(|E|)$ space. (Here, $|V|$ and $|E|$ refer to the number of vertices and edges of a graph.) It is difficult to overstate the significance of this development, as memory requirements at this stage were a severe, if not the defining, computational bottleneck. Thus, we only need space to store the grid decomposition of space rather than the entire mapping structure among those grid elements. For the problems we have been addressing, this amounts do being able to handle decompositions over 10-100 times the size; for maps with greater expansion the space savings will be even greater. Indeed, the theoretical worst case graph with $|E| = |V|^2$ can now be processed using only s$\mathcal{O}(V)$ memory, although we must be quick to point out the time requirement will still be $\mathcal{O}(|E|)$.

We have also implemented a succinct grid method to store $\mathcal{F}$ that allows us to work with graphs that consiste of several orders of magnitude more vertices. However, this comes at a computational cost. Both the modified Tarjan's algorithm and the succinct grid methods can be found in the latest database code [15]. Manuscripts providing details of these constructions are in progress.

4. *Construction of database.* The computational concepts and techniques described in topics 1 - 3 are all associated with dynamics near or at a single parameter value. One of the goals of the database is to provide information about the dynamics over large regions of parameter space. To do this we developed and implemented clutching records which gives information about how the dynamics changes between the regions [2]. More explicitly, for each region of parameter space a Morse Graph is computed. A clutching record gives a manner of comparing these two graphs. This information has a great deal of use. For example, it will have use in future applications where one seeks to form queries about the dynamics which track systems undergoing motion of their underlying parameters. Importantly, the clutching records may be used to create equivalence classes among the computed Morse sets. These equivalence classes are of importance because Conley index information computed for a single representative of the equivalence class holds for the entire continuation class. This is

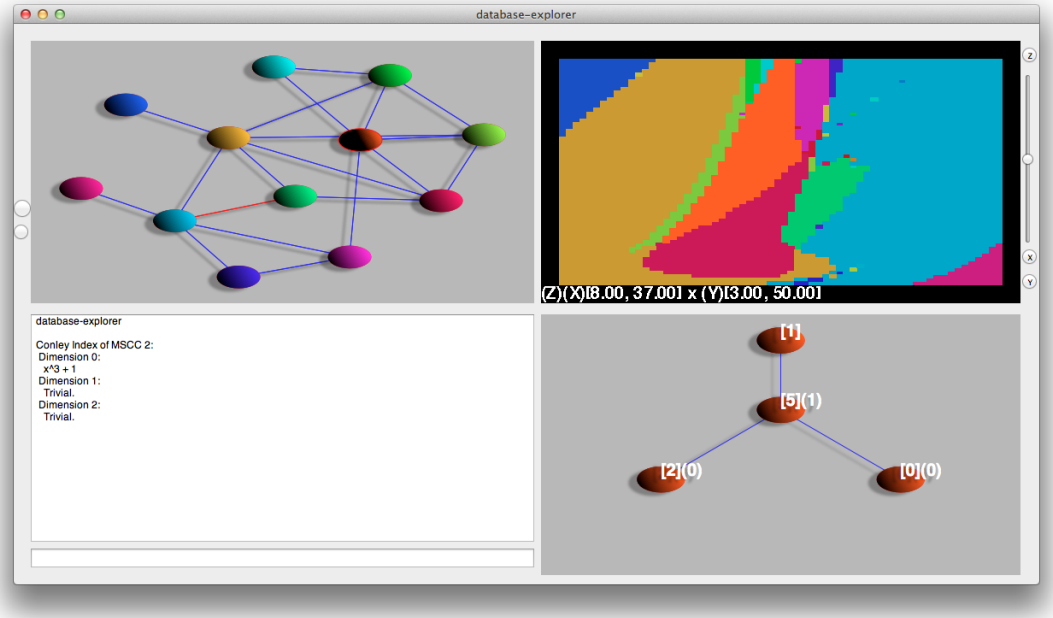


Figure 1: Screenshot of `database-explorer`

especially significant since the computation of the Conley index can be costly and in general Morse sets continue over large ranges of parameter space.

The data in the database is only as useful as our ability to visualize and query it. With this in mine we developed the database-explorer, which is software that can be used to visualize and explore the produced data.

Earlier versions of the database software [1] constructed a web page in a very specific manner requiring a large number of files – in particular every possible data request from a database had to be pre-rendered so it could be called up on demand by a `.php` script. This approach was rather inconvenient, not to mention wasteful of server disk space. The new approach using database-explorer is much simpler requiring only access to the single output file created by the database program after analyzing a dynamical system. In addition, the database-explorer allows one point-and-click access to the MGCC graph, highlighting relevant portions in parameter space. Also, one may inspect clutching information, which allows one to study bifurcations using our software in a way that was not previously possible.

We regard the database-explorer as a first step towards creating an interface for studying the database allowing a sophisticated range of queries.

5. *Efficient computation of homology.* As indicated above the database provides mathematically rigorous statements concerning global dynamics. The rigor is obtained by make use of algebraic topological invariants such as the Conley index. Thus the ability to perform efficient homological computations is central to this project.

   On the most fundamental level given a chain complex the associated homology is computed using the Smith Normal Form (SNF) of the boundary operator. Thus efficient computation of homology requires efficient algorithms for computing the SNF. At the moment the best worst case complexity analysis of the SNF algorithm gives a lower bound that is super cubical in the dimensions of the chain complex. We developed a preprocessing technique based on discrete Morse theory that provides a linear time reduction in the size of the original complex after which the SNF algorithm is applied [5, 6].

   The design of the Homology Software [15] has been refactored to allow for easier extension and more efficient processing. The improvements over the previous version have been incremental – the following list gives the highlights:

   (a) A simpler interface has been imposed on Cell Complex data structures using contiguous interfacing.

   (b) The code may now take any principal ideal domain as the underlying ring. This allows for computation under finite fields such as $\mathbb{Z}_2$, for example.

   (c) Shift Equivalence classes of matrices under a finite field may now be determined, allowing us to unambiguously state the Conley Index of isolating neighborhoods when dealing with finite fields.

   (d) The `Chain` class has been unified among all cell complexes, making it easier to understand and implement functions which communicate between different complexes.

   (e) We now employ a C++ technique known as *polymorphism* instead of *template design* whenever it does not produce an efficiency bottleneck to do so. This makes genericity in the code easier to achieve in a variety of situations.

   (f) The "Morse Complex", which allows efficient homology computation using Discrete Morse Theory, has been improved. In particular Morse complex boundaries are evalulated in a "lazy" fashion, meaning they are not computed unless required. This yields a performance boost in a settings where we use Discrete Morse Theory for tasks other than Homology computation (i.e. finding preboundaries of chains.)

   (g) The Map Homology algorithm has been optimized to no longer require the construction of the entire graph complex simultaneously.

(h) The chomp package is now *header-only*. This ensures the ability of the compiler to make any possible optimizations, while making it easier to install the package; they need only include the relevant header files.

The same preprocessing techniques have been applied to the computation of persistent homology [15, 16].

6. *Theoretical framework for database approach to dynamics.* It should be noted that the database approach provides a fundamentally different perspective to the analysis of nonlinear dynamics. While based to a large extent on the ideas of Conley from the early 70s, for the intended applications we are redeveloping the theory within an algorithmic and computational framework. This is a longer term effort but foundational results have been obtained [8].

7. *Alternative approaches.* While the primary focus of the grant was on developing topological methods for identifying global dynamics, we also considered methods for identifying and tracking particular structures and invariant sets based on analytic techniques [17, 18, 14].

8. *Applications of computational tools.* The computational tools described above provide new techniques for the analysis of high dimensional data. We applied these tools successfully to questions associated with Rayleigh-Benard convection [12, 13], dense granular media [11, 9, 10], and the compressibility of proteins [4].

# References


[1] Zin Arai, William D. Kalies, Hiroshi Kokubu, Konstantin Mischaikow, Hiroe Oka, and Paweł Pilarczyk. A database schema for the analysis of global dynamics of multiparameter systems. *SIAM J. Appl. Dyn. Syst.*, 8(3):757–789, 2009.

[2] Justin Bush, Marcio Gameiro, Shaun Harker, Hiroshi Kokubu, Konstantin Mischaikow, Ippei Obayashi, and Pawel Pilarczyk. Combinatorial-topological framework for the analysis of global dynamics. *CHAOS*, 22(4), DEC 2012.

[3] S. Ferry, K. Mischaikow, and V. Nanda. Reconstructing Functions from Random Samples. *Journal of Computational dynamics*, 2, 2014.

[4] M. Gameiro, Y. Hiraoka, S. Izumi, M. Kramar, K. Mischaikow, , and V. Nanda. Topological measurement of protein compressibility via persistence diagrams. *preprint*, 2014.

[5] S. Harker, K. Mischaikow, M. Mrozek, V. Nanda, H. Wagner, M. Juda, and P. Dlotko. The efficiency of a homology algorithm based on discrete morse theory and coreductions. In Rocio Gonzalez Diaz Pedro Real Jurado, editor, *Proceedings of the 3rd International Workshop on Computational Topology in Image Context, Chipiona, Spain, November 2010*, volume 3, pages 41–47. 2010.

[6] Shaun Harker, Konstantin Mischaikow, Marian Mrozek, and Vidit Nanda. Discrete morse theoretic algorithms for computing homology of complexes and maps. *Foundations of Computational Mathematics*, pages 1–34, 2013.

[7] William Kalies, Konstantin Mischaikow, and Robert C.A.M. Vandervorst. An algorithmic approach to chain recurrence. *Found. Comput. Math.*, 5(4):409–449, 2005.

[8] William Kalies, Konstantin Mischaikow, and Robert C.A.M. Vandervorst. Lattice Structures for Attractors I. *Journal of Computational dynamics*, 2, 2014.

[9] L. Kondic, A. Goullet, C.S. O'Hern, M. Kramar, K. Mischaikow, and R.P. Behringer. Topology of force networks in compressed granular media. *Europhys. Lett.*, 97:54001, 2012.

[10] M. Kramar, A. Goullet, L. Kondic, and K. Mischaikow. Persistence of force networks in compressed granular media. *Phys. Rev. E*, 87:042207, 2013.

[11] M. Kramar, A. Goullet, L. Kondic, and K. Mischaikow. Quantifying force networks in particulate systems. *ArXiv e-prints*, November 2013.

[12] H. Kurtuldu, K. Mischaikow, and M. F. Schatz. Measuring the departures from the Boussinesq approximation in Rayleigh-Benard convection experiments. *Journal of Fluid Mechanics*, 682:543–557, 2011.

[13] Hueseyin Kurtuldu, Konstantin Mischaikow, and Michael F. Schatz. Extensive Scaling from Computational Homology and Karhunen-Loeve Decomposition Analysis of Rayleigh-Benard Convection Experiments. *Physical Review Letters*, 107(3), 2011.

[14] J. D. Mireles James and Konstantin Mischaikow. Rigorous a posteriori computation of (un)stable manifolds and connecting orbits for analytic maps. *SIAM J. Appl. Dyn. Syst.*, 12(2):957–1006, 2013.

[15] K. Mischaikow. Computational Homology Project, http://chomp.rutgers.edu/.

[16] Konstantin Mischaikow and Vidit Nanda. Morse theory for filtrations and efficient computation of persistent homology. *Discrete Comput. Geom.*, 50(2):330–353, 2013.

[17] Jan Bouwe van den Berg, Jean-Philippe Lessard, and Konstantin Mischaikow. Global smooth solution curves using rigorous branch following. *Math. Comp.*, 79(271):1565–1584, 2010.

[18] Jan Bouwe van den Berg, Jason D. Mireles-James, Jean-Philippe Lessard, and Konstantin Mischaikow. Rigorous numerics for symmetric connecting orbits: even homoclinics of the Gray-Scott equation. *SIAM J. Math. Anal.*, 43(4):1557–1594, 2011.